STUDY OF THE CHEMICAL POTENTIAL CONCENTRATION DEPENDENCE FOR BINARY MIXTURES IN MOLECULAR DYNAMICS MODELS

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Modern molecular dynamics (MD) makes it possible to calculate thermodynamic quantities, including the chemical potential. This thermodynamic parameter determines the conditions of phase equilibrium in multicomponent systems.

In this work, MD models were produced for a number of binary liquid mixtures, including non-polar substances (benzene-toluene, hexane-cyclohexane, etc.) and aqueous solutions of several non-electrolytes. For each mixture, a series of models at various concentrations, including pure component models, were obtained. Subsequently, the chemical potential values of the components were calculated for these models using several approaches.

All approaches are based on the fluctuation theory. In the first method, the integral of the radial distribution function $g(r)$ is calculated, and its value at infinity is predicted. The resulting values G_{ij} allow for the calculation of the components' chemical potential according to Kirkwood-Buff theory. An additional method involves obtaining values from the structure factor $S(q)$ by extrapolating it to the limit $q \to 0$, with further calculations also carried out based on Kirkwood-Buff theory.

A geometric approach based on Voronoi volume statistics was also tested. In this approach, the Voronoi tessellation is calculated for the centers of molecules system for every single component. The Voronoi volume represents the volume per molecule in the mixture, and its average value is the inverse concentration. The variance of the distribution is directly related to concentration fluctuations and allows for their estimation within the MD model. The chemical potential calculation in this approach is carried out using fluctuation theory.

This work demonstrates the feasibility of calculating the chemical potential as a function of concentration for liquid mixtures and provides a comparison of several calculation methods, both classical and novel.